

ON THE INTEGRATION OF PRODUCTS OF WHITTAKER FUNCTIONS WITH RESPECT TO THE SECOND INDEX

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ABSTRACT. Several new formulas are developed that enable the evaluation of a family of definite integrals containing the product of two Whittaker $W_{\kappa, \mu}(x)$ -functions. The integration is performed with respect to the second index μ , and the first index κ is permitted to have any complex value, within certain restrictions required for convergence. The method utilizes complex contour integration along with various symmetry relations satisfied by the Whittaker functions. The new results derived in this paper are complementary to the previously known integrals of products of Whittaker functions, which generally treat integration with respect to either the first index κ or the primary argument x . A physical application involving radiative transport is discussed.

I. INTRODUCTION

Many problems in mathematical physics involve differential equations with solutions that can be expressed in terms of Whittaker's functions $W_{\kappa, \mu}(x)$ and $M_{\kappa, \mu}(x)$. Examples of the diverse applications include studies of the spectral evolution resulting from the Compton scattering of radiation by hot electrons,^{1,2,3} modeling of the structure of the hydrogen atom,⁴ analysis of the Schrödinger equation,⁵ studies of the Coulomb Green's function,⁶ and analysis of fluctuations in financial markets.⁷

In a number of applications, it is necessary to evaluate integrals of Whittaker functions. This need may arise out of the requirement to satisfy normalization or orthogonality conditions. In particular, in the analysis of time-dependent Compton scattering, it is necessary to evaluate integrals containing the product of two Whittaker $W_{\kappa, \mu}(x)$ -functions, where the variable of integration is the second index μ . This is an unusual situation that is not covered by any of the previously known formulas for integrals of products of Whittaker functions. The required integrals in the Compton scattering application are members of the general family

$$I(s) \equiv \int_0^\infty \frac{u \sinh(2\pi u) \Gamma(1/2 - \kappa - iu) \Gamma(1/2 - \kappa + iu)}{s + u^2} W_{\kappa, iu}(x) W_{\kappa, iu}(x_0) du, \quad (1)$$

where x and x_0 are real and positive, and s and κ are complex. This integral converges for all values of s in the complex plane, with the exclusion of the negative real semiaxis, provided that $\operatorname{Re} \kappa \neq \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$, if $\operatorname{Im} \kappa \neq 0$. It also converges in the special case $s = 0$, provided $\operatorname{Re} \kappa \neq \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$. In this paper we derive several exact formulas for the evaluation of the integral $I(s)$ that fully describe all of the convergent cases.

II. FUNDAMENTAL EQUATIONS

We shall begin by briefly reviewing some of the basic properties of the Whittaker functions that will be useful in our later work. The Whittaker functions $W_{\kappa, \mu}(z)$ and $M_{\kappa, \mu}(z)$ are confluent hypergeometric functions that are related to the Kummer functions $\Phi(a, b, z)$ and $\Psi(a, b, z)$ by^{8,9}

$$\begin{aligned} M_{\kappa, \mu}(z) &= z^{\mu+1/2} e^{-z/2} \Phi(1/2 + \mu - \kappa, 1 + 2\mu; z), \\ W_{\kappa, \mu}(z) &= z^{\mu+1/2} e^{-z/2} \Psi(1/2 + \mu - \kappa, 1 + 2\mu; z). \end{aligned} \quad (2)$$

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For small values of $|z|$, the function $M_{\kappa,\mu}(z)$ is given by the power series

$$M_{\kappa,\mu}(z) = e^{-z/2} z^{\mu+1/2} \sum_{n=0}^{\infty} \frac{(1/2 - \kappa + \mu)_n}{(1 + 2\mu)_n} \frac{z^n}{n!}, \quad (3)$$

where $(a)_n$ denotes the Pochhammer symbol, defined by⁹

$$(a)_n \equiv \frac{\Gamma(a+n)}{\Gamma(a)}. \quad (4)$$

The function $W_{\kappa,\mu}(z)$ can be expressed in terms of $M_{\kappa,\mu}(z)$ using⁸

$$W_{\kappa,\mu}(z) = \frac{\Gamma(-2\mu)}{\Gamma(1/2 - \mu - \kappa)} M_{\kappa,\mu}(z) + \frac{\Gamma(2\mu)}{\Gamma(1/2 + \mu - \kappa)} M_{\kappa,-\mu}(z). \quad (5)$$

The integrand in equation (1) for $I(s)$ is an even function of u , and therefore we can write

$$I(s) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{u \sinh(2\pi u) \Gamma(1/2 - \kappa - iu) \Gamma(1/2 - \kappa + iu)}{s + u^2} W_{\kappa,iu}(x) W_{\kappa,iu}(x_0) du. \quad (6)$$

Next we utilize (5) to express $W_{\kappa,iu}(x_0)$ as

$$W_{\kappa,iu}(x_0) = \frac{\Gamma(-2iu)}{\Gamma(1/2 - \kappa - iu)} M_{\kappa,iu}(x_0) + \frac{\Gamma(2iu)}{\Gamma(1/2 - \kappa + iu)} M_{\kappa,-iu}(x_0), \quad (7)$$

which can be rewritten as

$$\begin{aligned} W_{\kappa,iu}(x_0) &= \frac{\Gamma(-2iu) \Gamma(2iu)}{\Gamma(1/2 - \kappa - iu) \Gamma(1/2 - \kappa + iu)} \\ &\quad \times \left[\frac{\Gamma(1/2 - \kappa + iu)}{\Gamma(2iu)} M_{\kappa,iu}(x_0) + \frac{\Gamma(1/2 - \kappa - iu)}{\Gamma(-2iu)} M_{\kappa,-iu}(x_0) \right]. \end{aligned} \quad (8)$$

By employing the recurrence formula for the gamma function, $z \Gamma(z) = \Gamma(z+1)$, we can obtain the alternative form

$$\begin{aligned} W_{\kappa,iu}(x_0) &= \frac{\Gamma(-2iu) \Gamma(1+2iu)}{\Gamma(1/2 - \kappa - iu) \Gamma(1/2 - \kappa + iu)} \\ &\quad \times \left[\frac{\Gamma(1/2 - \kappa + iu)}{\Gamma(1+2iu)} M_{\kappa,iu}(x_0) - \frac{\Gamma(1/2 - \kappa - iu)}{\Gamma(1-2iu)} M_{\kappa,-iu}(x_0) \right]. \end{aligned} \quad (9)$$

Using this result to substitute for $W_{\kappa,iu}(x_0)$ in (6) now yields

$$\begin{aligned} I(s) &= \frac{1}{2} \int_{-\infty}^{\infty} \frac{u \sinh(2\pi u)}{s + u^2} \Gamma(-2iu) \Gamma(1+2iu) W_{\kappa,iu}(x) \\ &\quad \times \left[\frac{\Gamma(1/2 - \kappa + iu)}{\Gamma(1+2iu)} M_{\kappa,iu}(x_0) - \frac{\Gamma(1/2 - \kappa - iu)}{\Gamma(1-2iu)} M_{\kappa,-iu}(x_0) \right] du. \end{aligned} \quad (10)$$

By utilizing the reflection formula for the gamma function,

$$\Gamma(1+2iu) \Gamma(-2iu) = \frac{\pi i}{\sinh(2\pi u)}, \quad (11)$$

along with the symmetry relation [see Eq. (5)]

$$W_{\kappa,iu}(x) = W_{\kappa,-iu}(x), \quad (12)$$

we can rewrite (10) as

$$\begin{aligned} I(s) &= \frac{\pi i}{2} \int_{-\infty}^{\infty} \frac{u}{s + u^2} \left[\frac{\Gamma(1/2 - \kappa + iu)}{\Gamma(1+2iu)} W_{\kappa,iu}(x) M_{\kappa,iu}(x_0) \right. \\ &\quad \left. - \frac{\Gamma(1/2 - \kappa - iu)}{\Gamma(1-2iu)} W_{\kappa,-iu}(x) M_{\kappa,-iu}(x_0) \right] du. \end{aligned} \quad (13)$$

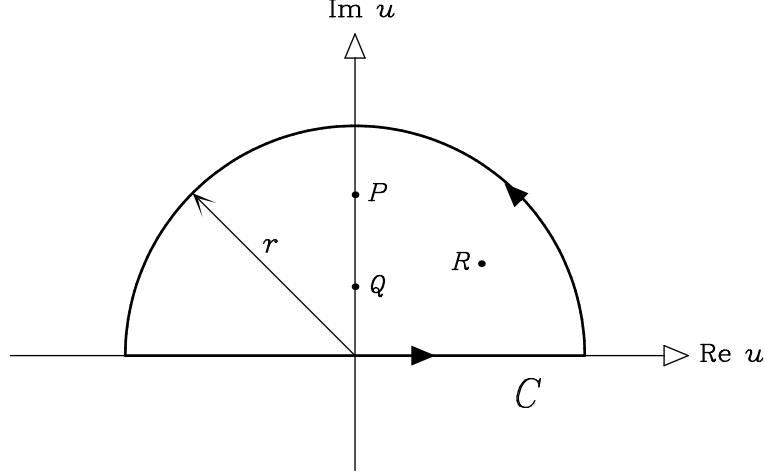


FIGURE 1. Integration around the closed contour C yields $I(s)$ in the limit $r \rightarrow \infty$ [see Eq. (16)]. In this example, κ is a real number in the range $3/2 < \kappa < 5/2$, and consequently there are two simple poles (P and Q) located inside the contour on the imaginary axis [see Eq. (18)]. The imaginary part of s is less than zero in this instance, and consequently there is also a simple pole, R , located at $u = i\sqrt{s}$ in quadrant I.

This relation can be split into two identical integrals, and consequently our expression for $I(s)$ can be reduced to

$$I(s) = -\pi i \int_{-\infty}^{\infty} \frac{u}{s+u^2} \frac{\Gamma(1/2 - \kappa - iu)}{\Gamma(1 - 2iu)} W_{\kappa, -iu}(x) M_{\kappa, -iu}(x_0) du . \quad (14)$$

III. CONTOUR INTEGRATION

The fundamental expression for the integral $I(s)$ given by (1) is clearly symmetrical with respect to the interchange of x and x_0 . We can use this flexibility to select the arguments of the W and M functions in such a way that the integration along the curved portion of the closed contour C in Fig. 1 vanishes in the limit $r \rightarrow \infty$. By employing asymptotic analysis, we find that this occurs if x_{\max} is the argument of the W function and x_{\min} is the argument of the M function, where

$$x_{\min} \equiv \min(x, x_0) , \quad x_{\max} \equiv \max(x, x_0) . \quad (15)$$

Equation (14) for $I(s)$ can therefore be recast as the complex contour integral

$$I(s) = \oint_C L(u) du , \quad (16)$$

where

$$L(u) \equiv -\pi i \frac{u}{s+u^2} \frac{\Gamma(1/2 - \kappa - iu)}{\Gamma(1 - 2iu)} W_{\kappa, -iu}(x_{\max}) M_{\kappa, -iu}(x_{\min}) . \quad (17)$$

We shall proceed to obtain an exact, closed form expression for $I(s)$ by utilizing the residue theorem to evaluate the integral in (16).

The integrand $L(u)$ has a simple pole located at $u = i\sqrt{s}$, where \sqrt{s} denotes the principle branch of the square root function. This pole is located in quadrant II of the complex u plane if $\text{Im } s \geq 0$, and otherwise it is located in quadrant I. In either case, the pole is contained within the closed integration contour C . Additional simple poles are located at the singularities of the function $\Gamma(1/2 - \kappa - iu)$, which occur where the quantity $1/2 - \kappa - iu$ is equal to zero or a negative integer. At least one of the poles falls in the upper half-plane if $\text{Re } \kappa > 1/2$. The poles are located at $u = u_n$, where

$$u_n \equiv i \left(\kappa - \frac{1}{2} - n \right) , \quad n = 0, 1, \dots, [\text{Re } \kappa - \frac{1}{2}] , \quad (18)$$

and $[a]$ indicates the integer part of a . Note that if $\mathcal{Re} \kappa < 1/2$, then only the pole at $u = i\sqrt{s}$ is contained within the contour C .

We can now use the residue theorem to write

$$I(s) = 2\pi i \sum_{n=0}^{[\mathcal{Re} \kappa - \frac{1}{2}]} \text{Res}(u_n) + 2\pi i \text{Res}(i\sqrt{s}) , \quad (19)$$

where $\text{Res}(u_*)$ denotes the residue associated with the simple pole located at $u = u_*$.

IV. EVALUATION OF THE RESIDUES

The residue corresponding to the simple pole at $u = i\sqrt{s}$ is easily computed using the formula

$$\text{Res}(i\sqrt{s}) = \lim_{u \rightarrow i\sqrt{s}} (u - i\sqrt{s}) L(u) , \quad (20)$$

which can be immediately evaluated to obtain

$$\text{Res}(i\sqrt{s}) = -\frac{\pi i}{2} \frac{\Gamma(1/2 - \kappa + \sqrt{s})}{\Gamma(1 + 2\sqrt{s})} W_{\kappa, \sqrt{s}}(x_{\max}) M_{\kappa, \sqrt{s}}(x_{\min}) . \quad (21)$$

Similarly, the residues associated with the simple poles located at $u = u_n$ are evaluated using

$$\text{Res}(u_n) = \lim_{u \rightarrow u_n} (u - u_n) L(u) . \quad (22)$$

Because the poles in this case correspond to the singularities of the function $\Gamma(1/2 - \kappa - iu)$, we will require evaluation of the quantity

$$\lim_{u \rightarrow u_n} (u - u_n) \Gamma\left(\frac{1}{2} - \kappa - iu\right) . \quad (23)$$

By combining (4) and (18) with the recurrence relation $z \Gamma(z) = \Gamma(z+1)$, we obtain

$$\Gamma\left(\frac{1}{2} - \kappa - iu\right) = \frac{\Gamma(1/2 - \kappa - iu + n)}{(1/2 - \kappa - iu)_n} = \frac{i \Gamma(1 + iu_n - iu)}{(iu_n - iu - n)_n (u - u_n)} , \quad (24)$$

and therefore

$$\lim_{u \rightarrow u_n} (u - u_n) \Gamma\left(\frac{1}{2} - \kappa - iu\right) = \frac{i(-1)^n}{n!} , \quad (25)$$

where we have used the fact that $(-n)_n = (-1)^n n!$. Next we need to evaluate the Whittaker functions appearing on the right-hand side of (17) in the limit $u \rightarrow u_n$. Using (2) and (18), we find that

$$\begin{aligned} M_{\kappa, -iu_n}(z) &= e^{-z/2} z^{\kappa-n} \Phi(-n, 2\kappa - 2n; z) , \\ W_{\kappa, -iu_n}(z) &= e^{-z/2} z^{\kappa-n} \Psi(-n, 2\kappa - 2n; z) . \end{aligned} \quad (26)$$

By employing equations (13.6.9) and (13.6.27) from Abramowitz and Stegun,⁹ we can rewrite these expressions as

$$\begin{aligned} M_{\kappa, -iu_n}(z) &= \frac{n!}{(\alpha + 1)_n} e^{-z/2} z^{(\alpha+1)/2} P_n^{(\alpha)}(z) , \\ W_{\kappa, -iu_n}(z) &= (-1)^n n! e^{-z/2} z^{(\alpha+1)/2} P_n^{(\alpha)}(z) , \end{aligned} \quad (27)$$

where $P_n^{(\alpha)}(z)$ denotes the Laguerre polynomial, and

$$\alpha \equiv 2\kappa - 2n - 1 = -2i u_n . \quad (28)$$

Combining (17), (22), (25), and (27), we obtain for the residue

$$\text{Res}(u_n) = \frac{2\pi i \alpha}{4s - \alpha^2} \frac{n!}{\Gamma(\alpha + n + 1)} e^{-(x+x_0)/2} (x x_0)^{(\alpha+1)/2} P_n^{(\alpha)}(x) P_n^{(\alpha)}(x_0) . \quad (29)$$

Utilizing this result along with (19) and (21), we conclude that

$$\begin{aligned}
I(s) &= \int_0^\infty \frac{u \sinh(2\pi u) \Gamma(1/2 - \kappa - iu) \Gamma(1/2 - \kappa + iu)}{s + u^2} W_{\kappa, iu}(x) W_{\kappa, iu}(x_0) du \\
&= \pi^2 \frac{\Gamma(1/2 - \kappa + \sqrt{s})}{\Gamma(1 + 2\sqrt{s})} W_{\kappa, \sqrt{s}}(x_{\max}) M_{\kappa, \sqrt{s}}(x_{\min}) \\
&\quad - 4\pi^2 e^{-(x+x_0)/2} \sum_{n=0}^{[\mathcal{R}e \kappa - \frac{1}{2}]} \frac{\alpha n!}{\Gamma(\alpha + n + 1)} \frac{(x x_0)^{(\alpha+1)/2}}{4s - \alpha^2} P_n^{(\alpha)}(x) P_n^{(\alpha)}(x_0),
\end{aligned} \tag{30}$$

where $\alpha = 2\kappa - 2n - 1$. This previously unknown integral formula is one of the main results of the paper. Note that the summation is carried out only if $\mathcal{R}e \kappa \geq 1/2$. The integral on the left-hand side of (30) converges for all complex values of s with the exception of the negative real semiaxis, provided that $\mathcal{R}e \kappa \neq \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$, if $\mathcal{I}m \kappa \neq 0$. When $s = 0$, the integral converges provided $\mathcal{R}e \kappa$ is not a positive half-integer.

A case of special interest can be generated by setting $x_0 = x$ in (30). The result obtained is the *quadratic normalization integral*,

$$\begin{aligned}
&\int_0^\infty \frac{u \sinh(2\pi u) \Gamma(1/2 - \kappa - iu) \Gamma(1/2 - \kappa + iu)}{s + u^2} W_{\kappa, iu}^2(x) du \\
&= \pi^2 \frac{\Gamma(1/2 - \kappa + \sqrt{s})}{\Gamma(1 + 2\sqrt{s})} W_{\kappa, \sqrt{s}}(x) M_{\kappa, \sqrt{s}}(x) \\
&\quad - 4\pi^2 e^{-x} \sum_{n=0}^{[\mathcal{R}e \kappa - \frac{1}{2}]} \frac{\alpha n!}{\Gamma(\alpha + n + 1)} \frac{x^{\alpha+1}}{4s - \alpha^2} \left[P_n^{(\alpha)}(x) \right]^2,
\end{aligned} \tag{31}$$

which is useful in situations involving the development of a series expansion in terms of a set of normalized basis functions. In the following sections, we shall proceed to discuss the limiting behavior of (30) observed when two of the poles coincide, as well as its relation to formulas appearing in the previous literature.

V. LIMITING BEHAVIOR

An interesting situation arises if the quantity $1/2 - \kappa + \sqrt{s}$ is equal to zero or a negative integer, because in this case the integral $I(s)$ converges, although the first term on the right-hand side of (30) formally *diverges* due to the appearance of the factor $\Gamma(1/2 - \kappa + \sqrt{s})$. This occurs when

$$\sqrt{s} = \sqrt{s_m} \equiv \kappa - \frac{1}{2} - m, \tag{32}$$

where m is a positive integer or zero. Since \sqrt{s} denotes the principle branch of the square root function, it follows that \sqrt{s} is located in either quadrants I or IV of the complex s plane, depending on whether $\mathcal{I}m s$ is positive or negative. Hence $\mathcal{R}e \sqrt{s} \geq 0$ in general, and therefore the function $\Gamma(1/2 - \kappa + \sqrt{s})$ has no singularities unless $\mathcal{R}e \kappa \geq 1/2$. The values of m yielding singularities for a given value of κ are

$$m = 0, 1, \dots, [\mathcal{R}e \kappa - \frac{1}{2}]. \tag{33}$$

When $s = s_m$, the divergence of the first term on the right-hand side of (30), containing the factor $\Gamma(1/2 - \kappa + \sqrt{s})$, is exactly balanced by the divergence of the $n = m$ term in the sum, leaving a finite residual quantity. This situation corresponds to a coincidence of the pole located at $u = i\sqrt{s}$ with the pole located at $u = u_m = i(\kappa - 1/2 - m)$ [see Eq. (18)]. In this case the resulting pole has order two. The associated residue can be computed by using the standard formula for a second-order pole, but it is more efficient to approach the calculation by evaluating equation (30) for $I(s)$ in the limit $s \rightarrow s_m$. The limiting value of the sum of the two divergent terms is given by

$$\begin{aligned}
K \equiv \lim_{s \rightarrow s_m} \pi^2 \frac{\Gamma(1/2 - \kappa + \sqrt{s})}{\Gamma(1 + 2\sqrt{s})} W_{\kappa, \sqrt{s}}(x_{\max}) M_{\kappa, \sqrt{s}}(x_{\min}) \\
- 4\pi^2 e^{-(x+x_0)/2} \frac{\lambda m!}{\Gamma(\lambda + m + 1)} \frac{(x x_0)^{(\lambda+1)/2}}{4s - \lambda^2} P_m^{(\lambda)}(x) P_m^{(\lambda)}(x_0),
\end{aligned} \tag{34}$$

where

$$\lambda \equiv 2\kappa - 2m - 1 = 2\sqrt{s_m} . \quad (35)$$

Equation (34) can be rewritten as

$$K = \lim_{s \rightarrow s_m} \frac{N}{D} , \quad (36)$$

where

$$\begin{aligned} N \equiv & \pi^2 (s - s_m) \frac{\Gamma(1/2 - \kappa + \sqrt{s})}{\Gamma(1 + 2\sqrt{s})} W_{\kappa, \sqrt{s}}(x_{\max}) M_{\kappa, \sqrt{s}}(x_{\min}) \\ & - \pi^2 e^{-(x+x_0)/2} \frac{\lambda m!}{\Gamma(\lambda + m + 1)} (x x_0)^{(\lambda+1)/2} P_m^{(\lambda)}(x) P_m^{(\lambda)}(x_0) , \end{aligned} \quad (37)$$

and

$$D \equiv s - s_m . \quad (38)$$

We can demonstrate that the numerator N vanishes in the limit $s \rightarrow s_m$ as follows. First we use (4) and (32) along with the recurrence relation for the gamma function to write

$$\Gamma\left(\frac{1}{2} - \kappa + \sqrt{s}\right) = \frac{\Gamma(1/2 - \kappa + \sqrt{s} + m)}{(1/2 - \kappa + \sqrt{s})_m} = \frac{(\sqrt{s} + \sqrt{s_m}) \Gamma(1 + \sqrt{s} - \sqrt{s_m})}{(s - s_m) (\sqrt{s} - \sqrt{s_m} - m)_m} , \quad (39)$$

and therefore [cf. Eq. (25)]

$$\lim_{s \rightarrow s_m} (s - s_m) \Gamma\left(\frac{1}{2} - \kappa + \sqrt{s}\right) = \frac{(-1)^m}{m!} 2\sqrt{s_m} . \quad (40)$$

Furthermore, based on (27), (28), and (35), we note that

$$\begin{aligned} M_{\kappa, \sqrt{s_m}}(z) &= \frac{m!}{(\lambda + 1)_m} e^{-z/2} z^{(\lambda+1)/2} P_m^{(\lambda)}(z) , \\ W_{\kappa, \sqrt{s_m}}(z) &= m! (-1)^m e^{-z/2} z^{(\lambda+1)/2} P_m^{(\lambda)}(z) . \end{aligned} \quad (41)$$

Taken together, (37), (40), and (41) indicate that the numerator N vanishes in the limit $s \rightarrow s_m$. The denominator D also vanishes in this limit, and therefore we can employ L'Hôpital's rule to evaluate K by writing

$$K = \lim_{s \rightarrow s_m} \frac{\partial N}{\partial s} \bigg/ \lim_{s \rightarrow s_m} \frac{\partial D}{\partial s} . \quad (42)$$

Since $\partial D / \partial s = 1$ and the second term on the right-hand side of (37) is independent of s , we obtain

$$K = \lim_{s \rightarrow s_m} \frac{\partial}{\partial s} \pi^2 (s - s_m) \frac{\Gamma(1/2 - \kappa + \sqrt{s})}{\Gamma(1 + 2\sqrt{s})} W_{\kappa, \sqrt{s}}(x_{\max}) M_{\kappa, \sqrt{s}}(x_{\min}) . \quad (43)$$

Upon differentiation, we obtain after a fairly lengthy calculation

$$K = \frac{\pi^2 e^{-(x+x_0)/2} (x x_0)^{(\lambda+1)/2} m! P_m^{(\lambda)}(x) P_m^{(\lambda)}(x_0)}{\Gamma(\lambda + m + 1)} \left[-\gamma_E + \frac{1}{\lambda} + H - 2\psi(\lambda + 1) - \frac{1}{m+1} + \sum_{n=1}^{m+1} \frac{1}{n} \right] , \quad (44)$$

where $\gamma_E \approx -0.577$ is Euler's constant, $\lambda = 2\kappa - 2m - 1$,

$$H \equiv \frac{\partial}{\partial \beta} \ln [W_{\kappa, \beta}(x_{\max}) M_{\kappa, \beta}(x_{\min})] \bigg|_{\beta=\sqrt{s_m}} , \quad (45)$$

and

$$\psi(z) \equiv \frac{d}{dz} \ln \Gamma(z) . \quad (46)$$

Combining results, we find that in the special case $s = s_m = (\kappa - m - 1/2)^2$ the integral $I(s)$ is given by

$$I(s) = \int_0^\infty \frac{u \sinh(2\pi u) \Gamma(1/2 - \kappa - iu) \Gamma(1/2 - \kappa + iu)}{(\kappa - m - 1/2)^2 + u^2} W_{\kappa, iu}(x) W_{\kappa, iu}(x_0) du$$

$$= K - 4\pi^2 e^{-(x+x_0)/2} \sum_{\substack{n=0 \\ n \neq m}}^{[\mathcal{R}e \kappa - \frac{1}{2}]} \frac{\alpha n!}{\Gamma(\alpha + n + 1)} \frac{(x x_0)^{(\alpha+1)/2}}{4s - \alpha^2} P_n^{(\alpha)}(x) P_n^{(\alpha)}(x_0), \quad (47)$$

where $\alpha = 2\kappa - 2n - 1$. The allowed range of values for m is given by (33), which indicates that we must have $\mathcal{R}e \kappa \geq 1/2$ in order for any of these special cases to occur. Note that the singular term with $n = m$ is not included in the sum, since that term is contained within K . Equations (30) and (47) cover all of the convergent cases of the fundamental integral $I(s)$. In Sec. VI we present simplified results obtained for certain values of the parameters.

VI. SPECIAL CASES

The general nature of the expression for $I(s)$ given by (30) encompasses many interesting special cases involving particular values for the parameters κ , s , x , and x_0 . In this section, we shall briefly discuss a few illustrative examples obtained when the first index κ is equal to an integer, in which case the general solution for $I(s)$ simplifies considerably. For brevity, we shall focus here on situations with $s \neq s_m$. However, we emphasize that formulas similar to those discussed below that are applicable to the case $s = s_m$ can also be obtained in a straightforward manner by starting with (47) rather than (30).

A. $\kappa = 0$

When $\kappa = 0$, the summation in (30) is not performed at all. Making use of the identities⁹

$$\Gamma\left(\frac{1}{2} - iu\right) \Gamma\left(\frac{1}{2} + iu\right) = \frac{\pi}{\cosh(\pi u)}, \quad (48)$$

and

$$\sinh(2\pi u) = 2 \sinh(\pi u) \cosh(\pi u), \quad (49)$$

we find that (30) reduces to

$$\int_0^\infty \frac{u \sinh(\pi u)}{s + u^2} W_{0, iu}(x) W_{0, iu}(x_0) du = \frac{\pi}{2} \frac{\Gamma(1/2 + \sqrt{s})}{\Gamma(1 + 2\sqrt{s})} W_{0, \sqrt{s}}(x_{\max}) M_{0, \sqrt{s}}(x_{\min}). \quad (50)$$

This result is convergent for all complex values of s , excluding the negative real semiaxis. Hence the point $s = 0$ is convergent in this case.

B. $\kappa = 1$

When $\kappa = 1$, there is one simple pole located at $s_0 = 1/4$, and we can make use of the identity

$$\Gamma\left(-\frac{1}{2} - iu\right) \Gamma\left(-\frac{1}{2} + iu\right) = \frac{4\pi}{\cosh(\pi u) (1 + 4u^2)}, \quad (51)$$

along with (49) to reduce (30) to the form

$$\int_0^\infty \frac{u \sinh(\pi u)}{(1 + 4u^2)(s + u^2)} W_{1, iu}(x) W_{1, iu}(x_0) du$$

$$= \frac{\pi}{8} \frac{\Gamma(\sqrt{s} - 1/2)}{\Gamma(1 + 2\sqrt{s})} W_{1, \sqrt{s}}(x_{\max}) M_{1, \sqrt{s}}(x_{\min}) - \frac{\pi}{2} \frac{x x_0 e^{-(x+x_0)/2}}{4s - 1}. \quad (52)$$

The right-hand side converges for all complex values of s with the exception of the point $s = 1/4$ [which must be treated using (47)] and the negative real semiaxis. The point $s = 0$ is convergent.

C. $\kappa = 2$

In this case there are two simple poles, located at $s_0 = 9/4$ and $s_1 = 1/4$. Utilizing the identity

$$\Gamma\left(-\frac{3}{2} - iu\right) \Gamma\left(-\frac{3}{2} + iu\right) = \frac{16\pi}{\cosh(\pi u) (9 + 4u^2) (1 + 4u^2)} , \quad (53)$$

along with (49), we can simplify (30) to obtain

$$\begin{aligned} & \int_0^\infty \frac{u \sinh(\pi u)}{(9 + 4u^2) (1 + 4u^2) (s + u^2)} W_{2, iu}(x) W_{2, iu}(x_0) du \\ &= \frac{\pi}{32} \frac{\Gamma(\sqrt{s} - 3/2)}{\Gamma(1 + 2\sqrt{s})} W_{2, \sqrt{s}}(x_{\max}) M_{2, \sqrt{s}}(x_{\min}) \\ & - \frac{\pi}{8} e^{-(x+x_0)/2} \sum_{n=0}^1 \frac{(3-2n) n!}{\Gamma(4-n)} \frac{(x x_0)^{2-n}}{4s - (3-2n)^2} P_n^{(3-2n)}(x) P_n^{(3-2n)}(x_0) . \end{aligned} \quad (54)$$

Evaluation of the Laguerre polynomials yields

$$\begin{aligned} & \int_0^\infty \frac{u \sinh(\pi u)}{(9 + 4u^2) (1 + 4u^2) (s + u^2)} W_{2, iu}(x) W_{2, iu}(x_0) du \\ &= \frac{\pi}{32} \frac{\Gamma(\sqrt{s} - 3/2)}{\Gamma(1 + 2\sqrt{s})} W_{2, \sqrt{s}}(x_{\max}) M_{2, \sqrt{s}}(x_{\min}) \\ & - \frac{\pi}{16} x x_0 e^{-(x+x_0)/2} \left[\frac{x x_0}{4s - 9} + \frac{(2-x)(2-x_0)}{4s - 1} \right] , \end{aligned} \quad (55)$$

which is convergent for all complex values of s , excluding the negative real semiaxis and the points $s = 1/4$, $s = 9/4$. These two points must be treated using (47). Note that the point $s = 0$ is convergent in this case. Similar results can be obtained for any positive or negative integer value of κ . The integral formula given by (55) is of particular significance in treating the scattering of radiation in an ionized plasma with a constant temperature, as discussed in Sec. VII.

VII. APPLICATION TO THERMAL COMPTONIZATION

One of the most important physical applications of the results developed in this paper involves the repeated Compton scattering of photons by a hot Maxwellian distribution of electrons with temperature T_e and number density n_e in an ionized plasma. This process, referred to as “thermal Comptonization,” is the primary mechanism responsible for the production of the radiation spectra observed from celestial X-ray sources such as active galaxies, black holes, and neutron stars.² When the electron temperature T_e is constant, the Green’s function, f_G , describing the temporal evolution of an initially monoenergetic radiation distribution satisfies the Kompaneets partial differential equation¹

$$\frac{\partial f_G}{\partial y} = \frac{1}{x^2} \frac{\partial}{\partial x} \left[x^4 \left(f_G + \frac{\partial f_G}{\partial x} \right) \right] , \quad (56)$$

where the dimensionless photon energy and the dimensionless time are denoted by

$$x(\epsilon) \equiv \frac{\epsilon}{kT_e} , \quad y(t) \equiv n_e \sigma_T c \frac{kT_e}{m_e c^2} (t - t_0) , \quad (57)$$

respectively, and the quantities ϵ , t_0 , t , σ_T , m_e , c , and k represent the photon energy, the initial time, the current time, the Thomson cross section, the electron mass, the speed of light, and Boltzmann’s constant, respectively. The terms proportional to f_G and $\partial f_G / \partial x$ inside the parentheses on the right-hand side of (56) express in turn the effects of electron recoil and stochastic (second-order Fermi) photon energization. At the initial time $t = t_0$, the radiation distribution is monoenergetic, and the Green’s function satisfies the initial condition

$$f_G(x, x_0, y) \Big|_{y=0} = x_0^{-2} \delta(x - x_0) , \quad (58)$$

where the dimensionless initial energy is given by

$$x_0 \equiv \frac{\epsilon_0}{kT_e} . \quad (59)$$

By operating on (56) with $\int_0^\infty x^2 dx$, we can establish that f_G has the convenient normalization

$$\int_0^\infty x^2 f_G(x, x_0, y) dx = \text{constant} = 1 , \quad (60)$$

where the final result follows from the initial condition [Eq. (58)]. Note that this normalization is maintained for all values of y , which reflects the fact that Compton scattering conserves photons. It can be shown based on (56) that the Laplace transform of the Green's function,

$$F(x, x_0, s) \equiv \int_0^\infty e^{-sy} f_G(x, x_0, y) dy , \quad (61)$$

is given by³

$$F(x, x_0, s) = x_0^{-2} x^{-2} e^{(x_0-x)/2} \frac{\Gamma(\mu-3/2)}{\Gamma(1+2\mu)} M_{2,\mu}(x_{\min}) W_{2,\mu}(x_{\max}) , \quad (62)$$

where the quantity μ is a function of the transform variable s , defined by

$$\mu(s) \equiv \left(s + \frac{9}{4}\right)^{1/2} , \quad (63)$$

and

$$x_{\min} \equiv \min(x, x_0) , \quad x_{\max} \equiv \max(x, x_0) . \quad (64)$$

The solution for the Green's function is obtained by performing the inverse Laplace transformation using the Mellin integral,

$$f_G(x, x_0, y) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{sy} F(x, x_0, s) ds , \quad (65)$$

where the real constant γ is chosen so that the line $\text{Re } s = \gamma$ lies to the right of the singularities in the integrand. By transforming the variable of integration from s to

$$s' \equiv s + \frac{9}{4} , \quad (66)$$

we can obtain the equivalent expression

$$f_G(x, x_0, y) = \frac{e^{-9y/4}}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{s'y} \tilde{F}(x, x_0, s') ds' , \quad (67)$$

where

$$\tilde{F}(x, x_0, s') \equiv x_0^{-2} x^{-2} e^{(x_0-x)/2} \frac{\Gamma(\sqrt{s'}-3/2)}{\Gamma(1+2\sqrt{s'})} M_{2,\sqrt{s'}}(x_{\min}) W_{2,\sqrt{s'}}(x_{\max}) . \quad (68)$$

The exact solution for the Green's function $f_G(x, x_0, y)$ can be obtained by taking the inverse Laplace transformation of (55), which yields

$$\begin{aligned} & \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{sy} \frac{\Gamma(\sqrt{s}-3/2)}{\Gamma(1+2\sqrt{s})} W_{2,\sqrt{s}}(x_{\max}) M_{2,\sqrt{s}}(x_{\min}) ds \\ &= \frac{32}{\pi} \int_0^\infty \frac{u \sinh(\pi u)}{(9+4u^2)(1+4u^2)} W_{2,iu}(x) W_{2,iu}(x_0) \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{sy}}{s+u^2} ds du \\ & \quad + \frac{xx_0}{2} e^{-(x+x_0)/2} \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{sy} \left[\frac{xx_0}{s-9/4} + \frac{(2-x)(2-x_0)}{s-1/4} \right] ds , \end{aligned} \quad (69)$$

where we have interchanged the order of integration in the double integral. The inverse Laplace transformations on the right-hand side of (69) are elementary in nature and can be evaluated using the formula

$$\frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{sy}}{s+k} ds = e^{-ky} . \quad (70)$$

By utilizing this result in (69), we obtain

$$\begin{aligned} \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{sy} \frac{\Gamma(\sqrt{s}-3/2)}{\Gamma(1+2\sqrt{s})} W_{2,\sqrt{s}}(x_{\max}) M_{2,\sqrt{s}}(x_{\min}) ds \\ = \frac{32}{\pi} \int_0^\infty e^{-u^2 y} \frac{u \sinh(\pi u)}{(9+4u^2)(1+4u^2)} W_{2,iu}(x) W_{2,iu}(x_0) du \\ + \frac{xx_0}{2} e^{-(x+x_0)/2} \left[xx_0 e^{9y/4} + (2-x)(2-x_0) e^{y/4} \right]. \end{aligned} \quad (71)$$

We can now combine (67), (68), and (71) to show that the exact solution for the time-dependent Green's function is given by³

$$\begin{aligned} f_G(x, x_0, y) = \frac{32}{\pi} e^{-9y/4} x_0^{-2} x^{-2} e^{(x_0-x)/2} \int_0^\infty e^{-u^2 y} \frac{u \sinh(\pi u)}{(1+4u^2)(9+4u^2)} \\ \times W_{2,iu}(x_0) W_{2,iu}(x) du + \frac{e^{-x}}{2} + \frac{e^{-x-2y}}{2} \frac{(2-x)(2-x_0)}{x_0 x}. \end{aligned} \quad (72)$$

Since the fundamental partial differential equation (56) is linear, the particular solution for the radiation distribution corresponding to an *arbitrary* initial spectrum can be found via convolution using the Green's function. The result given by (72) is therefore of central importance in the field of theoretical X-ray astronomy.

VIII. CONCLUSION

In this paper we have developed several new formulas for the evaluation of a family of integrals containing the product of two Whittaker $W_{\kappa,\mu}(x)$ -functions, when the integration occurs with respect to the second index μ , and that index is imaginary. The fundamental integral we have focused on in this paper is

$$I(s) \equiv \int_0^\infty \frac{u \sinh(2\pi u) \Gamma(1/2 - \kappa - iu) \Gamma(1/2 - \kappa + iu)}{s + u^2} W_{\kappa,iu}(x) W_{\kappa,iu}(x_0) du. \quad (73)$$

This is related to the Whittaker function index transformation discussed in Refs. 12 and 13. An expression of particular interest is the quadratic normalization integral given by (31). The results presented in (30) and (47) for $I(s)$ allow the exact evaluation of all of the convergent cases of this integral without the need to resort to numerical integration. We also point out that by utilizing equations (2), one can easily obtain a set of analogous integration formulas applicable to the Kummer functions $\Phi(a, b, z)$ and $\Psi(a, b, z)$. While integrals of this precise type have not been considered before, it is worth noting that $I(s)$ is a member of a wider group of integrals containing the product of two Whittaker W -functions. In general, the other integrals in this group involve integration with respect to one of the other parameters, rather than the second index as we have considered here. We briefly review a few of these related integrals below.

Several formulas are available in the previous literature for evaluating the integral of the product of two Whittaker $W_{\kappa,\mu}(x)$ -functions with respect to the primary argument x . For example, based upon equation (9.12) from Buchholz¹⁰ or equation (20.3.40) from Erdélyi et al.¹¹ or equation (7.611.3) from Gradshteyn and Ryzhik,⁸ we have

$$\begin{aligned} \int_0^\infty W_{\kappa,\mu}(x) W_{\sigma,\mu}(x) \frac{dx}{x} = \frac{1}{\kappa - \sigma} \frac{\pi}{\sin(2\pi\mu)} \left[\frac{1}{\Gamma(1/2 - \kappa + \mu) \Gamma(1/2 - \sigma - \mu)} \right. \\ \left. - \frac{1}{\Gamma(1/2 - \kappa - \mu) \Gamma(1/2 - \sigma + \mu)} \right], \end{aligned} \quad (74)$$

which is valid provided $|\operatorname{Re} \mu| < 1/2$. We note that the formulas in Refs. 8 and 11 are missing a factor of π , and the formula in Ref. 10 contains two incorrect signs. Another closely related example is given by equation (7.611.6) from Gradshteyn and Ryzhik⁸ or equation (20.3.41) from Ref. 11,

$$\int_0^\infty x^{\sigma-1} W_{\kappa,\mu}(x) W_{-\kappa,\mu}(x) dx = \frac{\Gamma(\sigma+1) \Gamma(\sigma/2 + 1/2 + \mu) \Gamma(\sigma/2 + 1/2 - \mu)}{2 \Gamma(\sigma/2 + 1 + \kappa) \Gamma(\sigma/2 + 1 - \kappa)}, \quad (75)$$

which is valid provided $\operatorname{Re} \sigma > 2|\operatorname{Re} \mu| - 1$.

A few formulas that treat the integration of a product of two Whittaker $W_{\kappa, \mu}(x)$ -functions with respect to the first index κ have also been known for some time. The most general expression is equation (15.10b) from Buchholz,¹⁰ which can be written as

$$\begin{aligned} \int_0^\infty \Gamma(k - iu) \Gamma(k + iu) W_{iu, k-1/2}(x) W_{-iu, k-1/2}(x_0) du \\ = \sqrt{\pi} \Gamma(2k) (x x_0)^k (x + x_0)^{-2k+1/2} K_{2k-1/2} \left(\frac{x + x_0}{2} \right), \end{aligned} \quad (76)$$

where $K_{2k-1/2}(z)$ denotes the modified Bessel function. When $k = 1/2$, this formula reduces to equation (7.691) from Ref. 8, which states that

$$\int_0^\infty \operatorname{sech}(\pi u) W_{iu, 0}(x) W_{-iu, 0}(x_0) du = \frac{\sqrt{x x_0}}{x + x_0} e^{-(x+x_0)/2}. \quad (77)$$

The new results for $I(s)$ obtained in this paper [Eqs. (30) and (47)] are in some sense complementary to these previously known formulas. We emphasize that the expressions developed here are of significance in a variety of applications, including the problem of the Comptonization of radiation in an isothermal plasma, discussed in Section VII. Our general approach may also allow the determination of the Green's function solution for the one-dimensional Schrödinger equation with the Morse potential.¹⁴ We plan to pursue this question in future work.

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